Diagrammatic analysis of the Hubbard model II: Superconducting state

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Diagrammatic analysis for normal state of Hubbard model proposed in our previous paper[1] is generalized and used to investigate superconducting state of this model. We use the notion of charge quantum number to describe the irreducible Green's function of the superconducting state. As in the previous paper we introduce the notion of tunneling Green's function and of its mass operator. This last quantity turns out to be equal to correlation function of the system. We proved the existence of exact relation between renormalized one-particle propagator and thermodynamic potential which includes integration over auxiliary interaction constant. The notion of skeleton diagrams of propagator and vacuum kinds were introduced. These diagrams are constructed from irreducible Green's functions and tunneling lines. Identity of this functional to the thermodynamic potential has been proved and the stationarity with respect to variation of the mass operator has been demonstrated.

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I. INTRODUCTION

The present paper generalizes our previous work[1] on diagrammatic analysis of the normal state of the Hubbard model[2−4] to the superconducting state.

Now we shall assume the existence of pairing of charge carriers and non-zero Bogolyubov quasi-averages[5] and, consequently, of the Gor'kov anomalous Green's functions[6].

The main property of the Hubbard model consists in the existence of strong electron correlations and, as a result, of the new diagrammatic elements with the structure of Kubo cumulants and named by us as irreducible Green's functions. These functions describe the main charge, spin and pairing fluctuations of the system.

The new diagram technique for such strongly correlated systems has been developed in our earlier papers[7 − 17]. This diagram technique uses the algebra of Fermi operators and relies on the generalized Wick theorem which contains, apart from usual Feynman contributions, additional irreducible structures. These structures are the main elements of the diagrams.

In superconducting state, unlike the normal one, the irreducible Green's functions can contain any even number of fermion creation and annihilation operators, whereas in normal state the number of both kinds is equal. Therefore we need an automatic mathematical mechanism which takes into account all the possibilities to consider the interference of the particles and holes in the superconducting state.

With this purpose we use the notion of charge quantum number, introduced by us in [7] and called $\alpha-$number, which has two values $\alpha = \pm 1$ according to the definition

$$C^{\alpha} = \begin{cases} C \;, & \alpha = 1; \\ C^{+}, & \alpha = -1. \end{cases} \tag{1}$$

Were C is a Fermion annihilation operator. In this new representation the tunneling part of the Hubbard Hamiltonian can be rewritten in the form

$$\begin{aligned} H' &= \sum_{\sigma} \sum_{\vec{x}\vec{x}'} t(\vec{x}' - \vec{x}) C^{+}_{\vec{x}'\sigma} C_{\vec{x}\sigma} \\ &= \frac{1}{2} \sum_{\alpha=-1,1} \sum_{\sigma} \sum_{\vec{x}\vec{x}'} \alpha t_{\alpha}(\vec{x}' - \vec{x}) C^{-\alpha}_{\vec{x}'\sigma} C^{\alpha}_{\vec{x}\sigma}, \end{aligned} \tag{2}$$

with the definition of the tunneling matrix elements

$$\begin{aligned} t_1(\vec{x}' - \vec{x}) &= t(\vec{x}' - \vec{x}) \\ t_{-1}(\vec{x}' - \vec{x}) &= t(\vec{x} - \vec{x}') \\ t(\vec{x} = 0) &= 0. \end{aligned} \tag{3}$$

In this charge quantum number representation the operator H' has an additional multiple α for every vertex of the diagrams and additional summation over α. All the Green's functions depend of this number.

In interaction representation operator H' has a form

$$\begin{aligned} H'(\tau) &= \frac{1}{2} \sum_{\alpha\sigma} \sum_{\vec{x}\vec{x}'} \alpha t_{\alpha}(\vec{x}' - \vec{x}) \\ &\times \; C^{-\alpha}_{\vec{x}'\sigma}(\tau + \alpha 0^{+}) C^{\alpha}_{\vec{x}\sigma}(\tau), \end{aligned} \tag{4}$$

The main part of the Hubbard Hamiltonian

$$\begin{aligned} H &= H^0 + H', \\ H^0 &= \sum_i H^0_i, \\ H^0_i &= -\mu \sum_{\sigma} C^{+}_{i\sigma} C_{i\sigma} + U n_{i\uparrow} n_{i\downarrow}, \end{aligned} \tag{5}$$

contains the local part H^0, where μ is the chemical potential and U is the Coulomb repulsion of the electrons.

This interaction is considered as a main parameter of the model and is taken into account in zero approximation of our theory. The operator H' describes electron hopping between lattice sites of the crystal and is considered as a perturbation.

We shall use the grand canonical partition function in our thermodynamic perturbation theory.

The paper is organized in the following way. In section II we determine the definition of one-particle Matsubara Green's functions by using α representation and develop the diagrammatic theory in the strong coupling limit.

In section III we establish relation between the full thermodynamic potential and the renormalized one-particle Green's function in the presence of additional integration over auxiliary constant of interaction λ and prove the stationarity theorem both for a special functional consisting of skeleton diagrams and for a renormalized thermodynamic potential shown to be its equivalent.

II. DIAGRAMMATIC THEORY

We shall use the following definition of the Matsubara Green's functions in the interaction representation

$$G^{\alpha\alpha'}(x|x') = -\left\langle TC^{\alpha}_{\overrightarrow{x}\sigma}(\tau)C^{-\alpha'}_{\overrightarrow{x}'\sigma'}(\tau')U(\beta)\right\rangle_0^c, \qquad (6)$$

where x stands for $(\overrightarrow{x},\sigma,\tau)$, index c of $\langle ...\rangle_0^c$ means the connected part of the diagrams and $\langle ...\rangle_0$ means thermal average with zero order partition function $\frac{e^{-\beta H^0}}{Tre^{-\beta H^0}}$.

We use the series expansion for the evolution operator $U(\beta)$ with some generalization because we introduce the auxiliary constant of interaction λ and use $\lambda H'$ instead H':

$$U_\lambda(\beta) \;=\; T\exp(-\lambda\int_0^\beta H'(\tau)d\tau), \qquad (7)$$

with T as the chronological operator. At the last stage of calculation this constant λ will be put equal to 1.

The correspondence between definition (6) and usual one [12] is the following:

$$\begin{aligned}
G^{1,1}_\lambda(x|x') &= -\left\langle TC_{\overrightarrow{x}\sigma}(\tau)\overline{C}_{\overrightarrow{x}'\sigma'}(\tau')U_\lambda(\beta)\right\rangle_0^c \\
&= G^\lambda_{\sigma,\sigma'}(\overrightarrow{x},\tau|\overrightarrow{x}',\tau'), \\
G^{1,-1}_\lambda(x|x') &= -\left\langle TC_{\overrightarrow{x}\sigma}(\tau)C_{\overrightarrow{x}'\sigma'}(\tau')U_\lambda(\beta)\right\rangle_0^c \\
&= F^\lambda_{\sigma,\overline{\sigma}'}(\overrightarrow{x},\tau|\overrightarrow{x}',\tau'), \qquad (8)\\
G^{-1,1}_\lambda(x|x') &= -\left\langle T\overline{C}_{\overrightarrow{x}\sigma}(\tau)\overline{C}_{\overrightarrow{x}'\sigma'}(\tau')U_\lambda(\beta)\right\rangle_0^c \\
&= \overline{F}^\lambda_{\overline{\sigma},\sigma'}(\overrightarrow{x},\tau|\overrightarrow{x}',\tau'), \\
G^{-1,-1}_\lambda(x|x') &= -G^{1,1}_\lambda(x'|x).
\end{aligned}$$

As a result of application of the Generalized Wick Theorem we obtain for propagator (6) the diagrammatic contributions depicted on the Fig.1 In superconducting state, unlike the normal state, the propagator lines do not contain arrows which determine the processes of creation and annihilation of electrons because indices α can take two values $\alpha = \pm 1$ and every vertex of the diagram describes different possibilities.

In Fig.1 the diagram a) is the zero order propagator, the diagram b) and more complicated diagrams of such kind are of chain type. They correspond to the contribution of the ordinary Wick theorem and give the Hubbard I approximation. The contributions of the diagrams c) and d) of Fig.1 are

$$\begin{aligned}
c) &= \frac{1}{2}\left\langle TC^{\alpha}_{\overrightarrow{x}}(\tau)C^{-\alpha_1}_{\overrightarrow{1}'}(\tau_1+\alpha_1 0^+)C^{\alpha_1}_{\overrightarrow{1}}(\tau_1)C^{-\alpha'}_{\overrightarrow{x}'}(\tau')\right\rangle_0^{ir} \\
&\times\; \alpha_1 t_{\alpha_1}(\overrightarrow{1}'-\overrightarrow{1}), \\
d) &= \frac{1}{2}\left\langle TC^{\alpha}_{\overrightarrow{x}}(\tau)C^{-\alpha_1}_{\overrightarrow{1}'}(\tau_1)C^{\alpha_2}_{\overrightarrow{2}}(\tau_2)C^{-\alpha'}_{\overrightarrow{x}'}(\tau')\right\rangle_0^{ir} \\
&\times\; \alpha_1 t_{\alpha_1}(\overrightarrow{1}'-\overrightarrow{1})\alpha_2 t_{\alpha_2}(\overrightarrow{2}'-\overrightarrow{2}) \\
&\times\; G^{(0)\alpha_1\alpha_2}(\overrightarrow{1},\tau_1|\overrightarrow{2}',\tau_2),
\end{aligned}$$

where $\langle ...\rangle_0^{ir}$ means the irreducible two-particle Green's function[2–5] and summation or integration is understood here and below when two repeated indices are present. Spin index has been omitted for simplicity. In the diagram c) the equality of lattice sites indices $\overrightarrow{x} = \overrightarrow{1}' = \overrightarrow{1} = \overrightarrow{x}'$ is assumed and in diagram d) $\overrightarrow{x} = \overrightarrow{1}' = \overrightarrow{2} = \overrightarrow{x}'$. The diagrams Fig.1 c), d) and e) contain irreducible two-particles Green's functions, depicted as the rectangles. In higher orders of perturbation theory more complicated many-particle irreducible Green's functions $G^{(0)ir}_n[1,2,...,n]$ appear. These functions are local, i.e. with equal lattice site indices. Therefore the diagram c) in Fig.1 can be dropped since it contains a vanishing matrix element, $t(\overrightarrow{x}-\overrightarrow{x}) = 0$. The process of renormalization of the tunneling amplitude shown in the diagrams c) and d) leads to the replacement of the bare tunneling matrix element $\alpha t_\alpha(\overrightarrow{x}'-\overrightarrow{x})$ in c) by a renormalized quantity $T^{\alpha'\alpha}(x'|x)$. This process is determined by the equation

$$\begin{aligned}
T^{\alpha'\alpha}_{\sigma'\sigma}(x'|x) &= T^{(0)\alpha'\alpha}_{\sigma'\sigma}(x'|x) + T^{(0)\alpha'\alpha_1}_{\sigma'\sigma_1}(x'|x_1) \qquad (9)\\
&\times\; G^{\alpha_1\alpha_2}_{\sigma_1\sigma_2}(x_1|x_2)T^{(0)\alpha_2\alpha}_{\sigma_2\sigma}(x_2|x),
\end{aligned}$$

where

$$T^{(0)\alpha'\alpha}_{\sigma'\sigma}(x'|x) \;=\; \delta_{\alpha\alpha'}\alpha t_\alpha(\overrightarrow{x}'-\overrightarrow{x})\delta(\tau'-\tau-\alpha 0^+)\delta_{\sigma\sigma'}, \qquad (10)$$

and $G^{\alpha_1\alpha_2}$ is the full one-particle propagator. The quantity $T^{\alpha'\alpha}$ is shown in the diagrams as a double dashed line.

We then introduce the notion of correlation function $\Lambda^{\alpha\alpha'}(x|x')$ which is the infinite sum of strongly connected parts of propagator's diagrams. If we now omit from these diagrams all those contained in the process of renormalization of the tunneling matrix element, we obtain

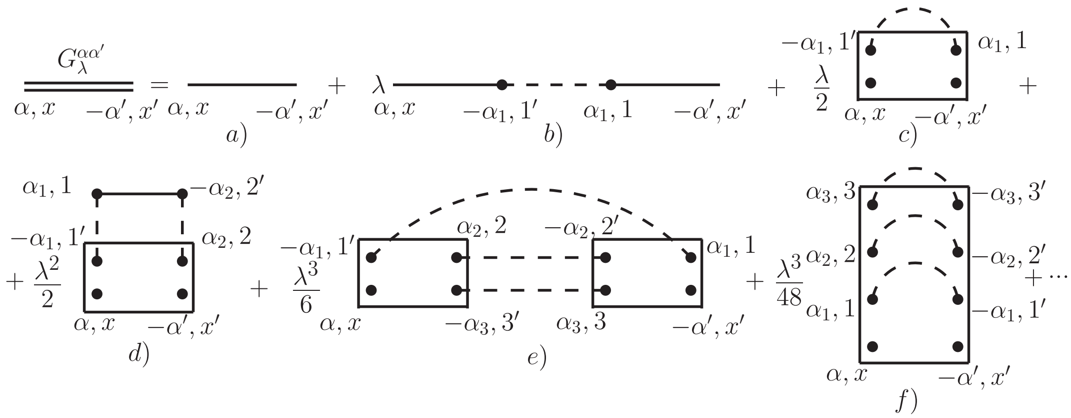

FIG. 1: The examples of the first orders perturbation theory diagrams for propagator. Solid thin lines depict zero order one-particle Green's functions and rectangles depict two- and four-particle irreducible Green's functions. Thin dashed lines correspond to tunneling matrix elements. Double solid line corresponds to renormalized propagator.

the skeleton diagrams for correlation function. In such skeleton diagrams we replace thin dashed lines by double dashed lines and obtain the definition of $\Lambda^{\alpha\alpha'}(x|x')$ shown in the Fig.2

There are two kinds of λ dependence in the diagrams of Fig.2. One is conditioned by dependence of $T_\lambda^{\alpha\alpha'}$ and the second is determined by λ being an explicit prefactor in the diagrams. In Hubbard I approximation only the free propagator line is taken into account. All the contributions of Fig.2 except the last one are local and their Fourier representation is independent of momentum. Only these diagrams are taken into account in Dynamical Mean Field Theory[18]. The last diagram of Fig.2 has the Fourier representation which depends of momentum.

As a result of diagrammatic analysis we can formulate the Dyson-type equation for full one-particle Green's function ($x = \overrightarrow{x}, \tau$):

$$\begin{aligned} G_{\sigma\sigma'}^{\alpha\alpha'}(x|x') &= \Lambda_{\sigma\sigma'}^{\alpha\alpha'}(x|x') + \sum_{\sigma_1\sigma_2} \sum_{\overrightarrow{x}_1 \overrightarrow{x}_2} \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 \\ &\times \Lambda_{\sigma\sigma_1}^{\alpha\alpha_1}(x|x_1) T_{\sigma_1\sigma_2}^{(0)\alpha_1\alpha_2}(x_1|x_2) G_{\sigma_2\sigma'}^{\alpha_2\alpha'}(x_2|x'). \end{aligned} \tag{11}$$

This equation can be written in the operator form:

$$\widehat{G} = (1 - \widehat{\Lambda}\widehat{T}^0)^{-1}\widehat{\Lambda} = \widehat{\Lambda}(1 - \widehat{T}^0\widehat{\Lambda})^{-1} \tag{12}$$

Using equations (9) and (12) we obtain the Dyson equation for the tunneling Green's function

$$\widehat{T} = \widehat{T}^0(1 - \widehat{\Lambda}\widehat{T}^0)^{-1} = (1 - \widehat{T}^0\widehat{\Lambda})^{-1}\widehat{T}^0, \tag{13}$$

where the correlation function Λ has the role of mass operator for the renormalized tunneling Green's function.

In Appendix A we demonstrate the equivalence of the equation (11) to usual[6] representation of superconducting Green's functions.

III. THERMODYNAMIC POTENTIAL DIAGRAMS

The thermodynamic potential of the system is determined by the connected part of the mean value of evolution operator:

$$F(\lambda) = F_0 - \frac{1}{\beta} \langle U_\lambda(\beta) \rangle_0^c, \tag{14}$$

with λ equal to 1.

In the Fig.3 are depicted the first order diagrams for $\langle U_\lambda(\beta) \rangle_0^c$.

The notations in Fig.3 are $n = (\overrightarrow{n}, \tau_n)$ and $n' = (\overrightarrow{n}', \tau_n + \alpha_n 0^+)$.

The first three diagrams in Fig.3 are of chain type and correspond to the Hubbard I approximation. The next diagrams contain the rectangles which represent our irreducible Green's functions. Indeed, some of these diagrams are equal to zero when the dashed lines are self-closed by virtue of the relation $t(0) = 0$. However, when these dashed lines are replaced by renormalized quantities T_λ their contributions are different from zero and should be retained. Such renormalized tunneling quantities will be used in the next part of the paper. The contributions of the fifth and eighth diagrams on the right-hand side of Fig.3 are

$$\begin{aligned} &- \frac{1}{4} \left\langle TC_{\overrightarrow{1}}^{\alpha_1}(\tau_1) C_{\overrightarrow{2}'}^{-\alpha_2}(\tau_2) C_{\overrightarrow{3}}^{\alpha_3}(\tau_3) C_{\overrightarrow{1}'}^{-\alpha_1}(\tau_1 + \alpha_1 0^+) \right\rangle_0^{ir} \\ &\times\ \alpha_1 t_{\alpha_1}(\overrightarrow{1}' - \overrightarrow{1}) \alpha_2 t_{\alpha_2}(\overrightarrow{2}' - \overrightarrow{2}) \alpha_3 t_{\alpha_3}(\overrightarrow{3}' - \overrightarrow{3}) \\ &\times\ G^{(0)\alpha_2\alpha_3}(\overrightarrow{2}, \tau_2 | \overrightarrow{3}', \tau_3), \\ &+\ \frac{1}{48} \left\langle TC_{\overrightarrow{1}}^{\alpha_1}(\tau_1) C_{\overrightarrow{2}'}^{-\alpha_2}(\tau_2) C_{\overrightarrow{3}}^{\alpha_3}(\tau_3) C_{\overrightarrow{4}'}^{-\alpha_4}(\tau_4) \right\rangle_0^{ir} \\ &\times\ \alpha_1 t_{\alpha_1}(\overrightarrow{1}' - \overrightarrow{1}) \alpha_2 t_{\alpha_2}(\overrightarrow{2}' - \overrightarrow{2}) \\ &\times\ \left\langle TC_{\overrightarrow{4}}^{\alpha_4}(\tau_4) C_{\overrightarrow{3}'}^{-\alpha_3}(\tau_3) C_{\overrightarrow{2}}^{\alpha_2}(\tau_2) C_{\overrightarrow{1}'}^{-\alpha_1}(\tau_1) \right\rangle_0^{ir} \\ &\times\ \alpha_3 t_{\alpha_3}(\overrightarrow{3}' - \overrightarrow{3}) \alpha_4 t_{\alpha_4}(\overrightarrow{4}' - \overrightarrow{4}), \end{aligned}$$

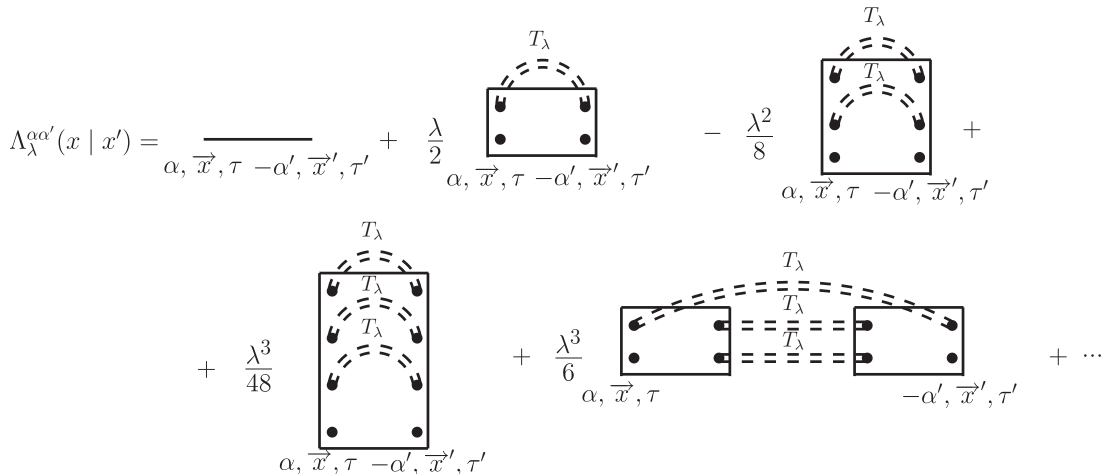

FIG. 2: The skeleton diagrams for correlation function $\Lambda^{\alpha\alpha'}(x|x')$. The rectangles depict the many-particles irreducible Green's function. The double dashed lines depict the full tunneling Green function $T_\lambda^{\alpha\alpha'}(x|x')$.

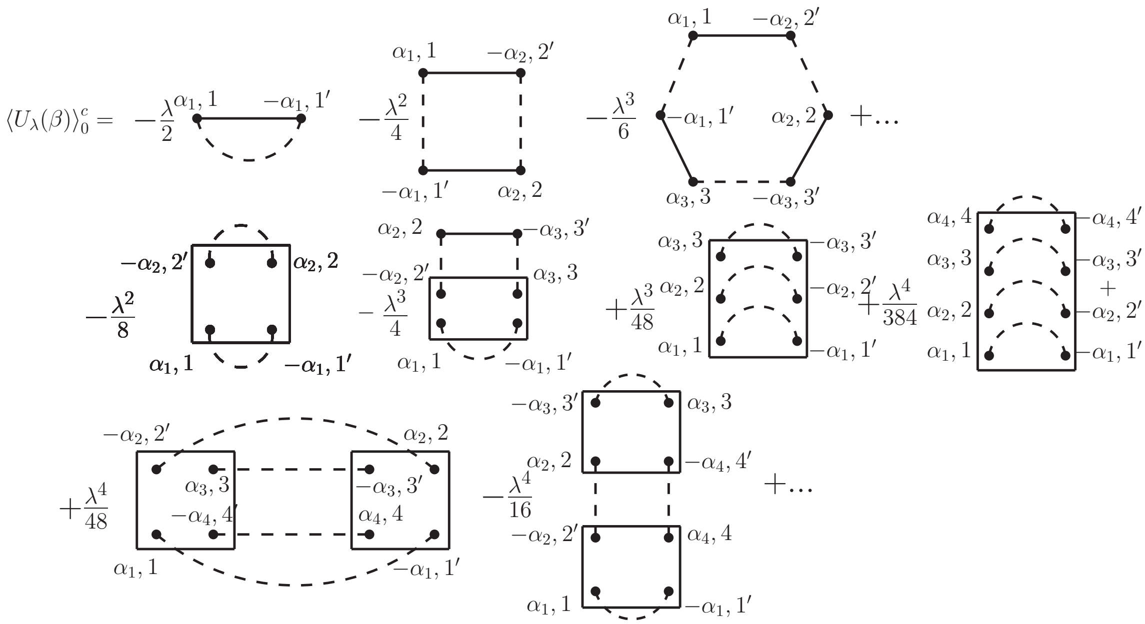

FIG. 3: The first orders of perturbation theory contributions.

respectively.

Comparison of the diagrams of Fig.1 for the $G^{(n)\alpha\alpha'}$ (n-th order of perturbation theory for the one-particle propagator) to the contributions of Fig.2 for $\left\langle U_\lambda^{n+1}(\beta)\right\rangle_0^c$ ($(n+1)$-th order for evolution operator) allows us to establish the following simple relation ($n \geq 1$):

$$
\begin{aligned}
\left\langle U_\lambda^{(n+1)}(\beta)\right\rangle_0^c &= -\frac{\beta}{2}\int\limits_0^\lambda \frac{d\lambda_1}{\lambda_1} \sum_{\overrightarrow{1}\,\overrightarrow{1}'} \sum_{\alpha_1\sigma_1} \lambda_1 \alpha_1 t_{\alpha_1}(\overrightarrow{1}' - \overrightarrow{1}) \\
&\times \; G_{\sigma_1\lambda_1}^{(n)\alpha_1\alpha_1}(\overrightarrow{1} - \overrightarrow{1}' | -\alpha_1 0^+),
\end{aligned}
$$

and as the result we have

$$
\begin{aligned}
\langle U_\lambda(\beta)\rangle_0^c &= -\frac{1}{2}\int\limits_0^\lambda \frac{d\lambda_1}{\lambda_1}\beta \sum_{\overrightarrow{1}\,\overrightarrow{1}'} \sum_{\alpha_1\sigma_1} \lambda_1\alpha_1 t_{\alpha_1}(\overrightarrow{1}' - \overrightarrow{1}) \\
&\times \; G_{\sigma_1\lambda_1}^{\alpha_1\alpha_1}(\overrightarrow{1} - \overrightarrow{1}' | -\alpha_1 0^+) \qquad (15) \\
&= -\frac{1}{2}\int\limits_0^\lambda \frac{d\lambda_1}{\lambda_1} Tr(\lambda_1 \widehat{T}^0 \widehat{G}_{\lambda_1}).
\end{aligned}
$$

Taking into account equations (12) and (13) we obtain

$$
\langle U_\lambda(\beta)\rangle_0^c = -\frac{1}{2}\int\limits_0^\lambda \frac{d\lambda_1}{\lambda_1} Tr(\lambda_1 \widehat{T}_{\lambda_1} \widehat{\Lambda}_{\lambda_1}). \qquad (16)
$$

Then from (14) and (16) it follows that

$$F(\lambda) = F_0 + \frac{1}{2\beta}\int_0^\lambda \frac{d\lambda_1}{\lambda_1} Tr(\lambda_1 \widehat{T}_{\lambda_1}\widehat{\Lambda}_{\lambda_1}) = F_0 + \frac{1}{2\beta}\int_0^\lambda \frac{d\lambda_1}{\lambda_1} Tr(\widehat{T}_{\lambda_1}\widehat{\Sigma}_{\lambda_1}), \quad (17)$$

where

$$\widehat{\Sigma}_\lambda = \lambda\widehat{\Lambda}_\lambda \quad (18)$$

has the role of mass operator for tunneling Green's function $\widehat{T}_\lambda$. For them Dyson equation exists:

$$\widehat{T} = \widehat{T}^0 + \widehat{T}^0\widehat{\Sigma}\widehat{T}. \quad (19)$$

Equation (17) can be rewritten in the form

$$\lambda\frac{dF(\lambda)}{d\lambda} = \frac{1}{2\beta}Tr(\widehat{T}_\lambda\widehat{\Sigma}_\lambda). \quad (20)$$

The equations (15) and (17) establish the relation between the thermodynamic potential and renormalized one-particle propagator $\widehat{G}_\lambda$ or tunneling Green's function $\widehat{T}_\lambda$. Both these quantities depend on auxiliary parameter λ which is integrated over. As have been proved by Luttinger and Ward[19,20], for normal state of weakly correlated systems, it is possible to obtain another expression for the thermodynamic potential without such additional integration.

In our previous paper[1], for the normal state of Hubbard model, we have obtained such an equation in the form of special functional. We now consider its generalization to the case of superconductivity. For this purpose we introduce the functional

$$Y(\lambda) = Y_1(\lambda) + Y'(\lambda), \quad (21)$$

where

$$Y_1(\lambda) = -\frac{1}{2}Tr\{\ln(\lambda\widehat{T}^0\widehat{\Lambda}_\lambda - 1) + \widehat{T}_\lambda\lambda\widehat{\Lambda}_\lambda\}, \quad (22)$$

and $Y'(\lambda)$ is the functional constructed from skeleton diagrams depicted on Fig.4.

From Fig.4 and Fig.2 it is possible to obtain the relation

$$\frac{\delta Y'(\lambda)}{\delta T_\lambda^{\alpha\alpha'}(x|x')} = \frac{1}{2}\lambda\Lambda_\lambda^{\alpha'\alpha}(x'|x). \quad (23)$$

Now we shall take into account the following functional derivatives based on the equation (12) and (13):

$$\frac{\delta}{\delta T_\lambda^{\alpha\alpha'}(x|x')}Tr(\ln(\widehat{T}^0\widehat{\Lambda}\lambda - 1)) = -Tr(\widehat{T}\frac{\delta\widehat{\Lambda}}{\delta T_\lambda^{\alpha\alpha'}(x|x'}),$$
$$\frac{\delta}{\delta T_\lambda^{\alpha\alpha'}(x|x')}Tr(\widehat{T}\widehat{\Lambda}\lambda) = \lambda\Lambda_\lambda^{\alpha'\alpha}(x'|x) + Tr(\widehat{T}_\lambda\frac{\delta\widehat{\Lambda}_\lambda}{\delta T_\lambda^{\alpha\alpha'}(x|x'}\lambda). \quad (24)$$

As a consequence of these equations we have

$$\frac{\delta}{\delta T_\lambda^{\alpha\alpha'}(x|x')}Tr\{\ln(\lambda\widehat{T}^0\widehat{\Lambda}_\lambda - 1) + \lambda\widehat{T}_\lambda\widehat{\Lambda}_\lambda\} = \lambda\Lambda_\lambda^{\alpha'\alpha}(x'|x), \quad (25)$$

and

$$\frac{\delta Y_1(\lambda)}{\delta T_\lambda^{\alpha\alpha'}(x|x')} = -\frac{\lambda}{2}\Lambda_\lambda^{\alpha'\alpha}(x'|x). \quad (26)$$

With the functional derivative of $Y'(\lambda)$ given in (23) we obtain the stationarity property of the functional $Y(\lambda)$:

$$\frac{\delta Y(\lambda)}{\delta T_\lambda^{\alpha\alpha'}(x|x')} = 0 \quad (27)$$

Using the definition (18) of the mass operator $\widehat{\Sigma}_\lambda$ we can rewrite the functional $Y_1(\lambda)$ in the form

$$Y_1(\lambda) = -\frac{1}{2}Tr\{\ln(\widehat{T}^0\widehat{\Sigma}_\lambda - 1) + \widehat{T}_\lambda\widehat{\Sigma}_\lambda\}, \quad (28)$$

and prove the second form of stationarity property

$$\frac{\delta\ Y(\lambda)}{\delta\widehat{\Sigma}_\lambda} = 0. \quad (29)$$

To demonstrate this equation it is sufficient to use the Dyson equation (19) in the form

$$\widehat{T^0}^{-1} = \widehat{T}_\lambda^{-1} + \widehat{\Sigma}_\lambda, \quad (30)$$

and the derivatives:

$$\frac{\delta(\widehat{T}_\lambda^{-1})^{\beta\beta'}(y|y')}{\delta(\widehat{\Sigma}_\lambda)^{\alpha\alpha'}(x|x')} = \delta_{\alpha\beta}\delta_{\alpha'\beta'}\delta_{xy}\delta_{x'y'},$$
$$\frac{\delta(\widehat{T}_\lambda)^{\beta\beta'}(y|y')}{\delta(\widehat{\Sigma}_\lambda)^{\alpha\alpha'}(x|x')} = (\widehat{T}_\lambda)^{\alpha'\beta'}(x'|y')(\widehat{T}_\lambda)^{\beta\alpha}(y|x),$$
$$\frac{\delta}{\delta(\widehat{\Sigma}_\lambda)^{\alpha\alpha'}(x|x')}Tr(\widehat{T}_\lambda\widehat{\Sigma}_\lambda) = (\widehat{T}_\lambda)^{\alpha'\alpha}(x'|x) + (\widehat{T}_\lambda\widehat{\Sigma}_\lambda\widehat{T}_\lambda)^{\alpha'\alpha}(x'|x), \quad (31)$$
$$\frac{\delta}{\delta(\widehat{\Sigma}_\lambda)^{\alpha\alpha'}(x|x')}Tr\{\ln(\widehat{T}^0\widehat{\Sigma}_\lambda - 1)\} = -(\widehat{T}_\lambda)^{\alpha'\alpha}(x'|x).$$

Therefore we have

$$\frac{\delta Y_1(\lambda)}{\delta(\widehat{\Sigma}_\lambda)^{\alpha\alpha'}(x|x')} = -\frac{1}{2}(\widehat{T}_\lambda\widehat{\Sigma}_\lambda\widehat{T}_\lambda)^{\alpha'\alpha}(x'|x), \quad (32)$$

and

$$\frac{\delta Y'(\lambda)}{\delta(\widehat{\Sigma}_\lambda)^{\alpha\alpha'}(x|x')} = \frac{\delta Y'(\lambda)}{\delta(\widehat{T}_\lambda)^{\beta\beta'}(y|y')}\frac{\delta(\widehat{T}_\lambda)^{\beta\beta'}(y|y')}{\delta(\widehat{\Sigma}_\lambda)^{\alpha\alpha'}(x|x')} = \frac{1}{2}(\widehat{T}_\lambda\widehat{\Sigma}_\lambda\widehat{T}_\lambda)^{\alpha'\alpha}(x'|x), \quad (33)$$

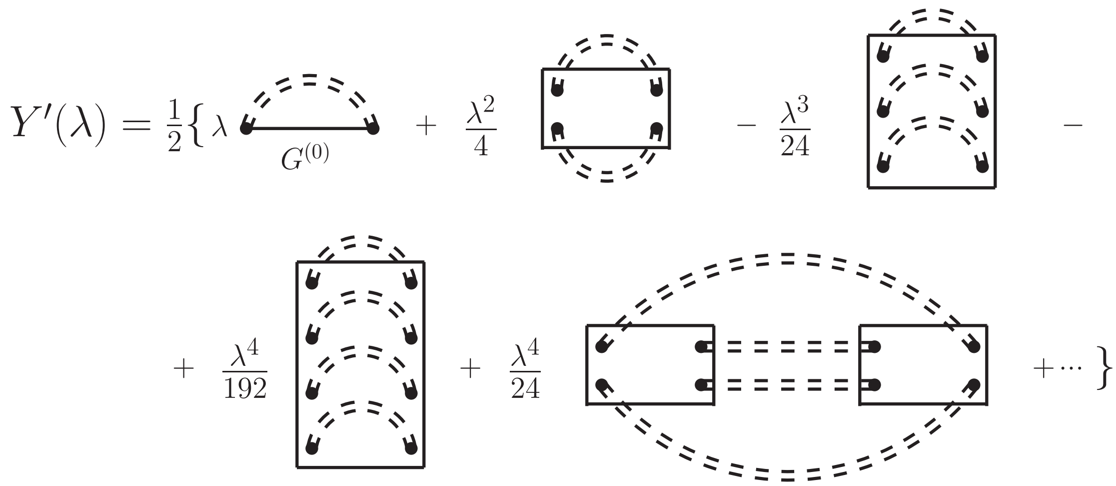

FIG. 4: The skeleton diagrams for functional $Y'(\lambda)$. The rectangles depict the irreducible Green's functions. The double dashed lines depict the tunneling renormalized Green's functions $T^{\alpha\alpha'}(x|x')$.

where the usual convention about summation over the repeated indices has been adopted.

As a result we obtain the stationarity property (29) of the functional $Y(\lambda)$ versus the change of the mass operator Σ_λ. This mass operator for $\lambda = 1$ coincides with correlation function of our strongly correlated model.

Now it is necessary to find a relation between the thermodynamic potential $F(\lambda)$ and the functional $Y(\lambda)$.

Consider first the value of the derivative $\frac{dY(\lambda)}{d\lambda}$. The λ dependence of the functional $Y(\lambda)$ is of two kinds: through Σ_λ and also explicit through the factors λ^n in front of the skeleton diagrams for the functional $Y'(\lambda)$.

Due the stationarity property (29) we obtain

$$\begin{aligned} \frac{dY(\lambda)}{d\lambda} &= \frac{\delta Y(\lambda)}{\delta \Sigma_\lambda}\frac{d\Sigma_\lambda}{d\lambda} + \frac{\partial Y(\lambda)}{\partial \lambda}|_{\Sigma_\lambda} \\ &= \frac{dY(\lambda)}{d\lambda}|_{\Sigma_\lambda} = \frac{dY'(\lambda)}{d\lambda}|_{\Sigma_\lambda}. \end{aligned} \tag{34}$$

Here we took into account that the $Y_1(\lambda)$ part of functional $Y(\lambda)$ (see equations (21) and (28)) does not explicitly dependent on λ.

By using the definitions of $Y'(\lambda)$ (see Fig.4) and of Λ_λ (see Fig. 2) it is easy to establish the property:

$$\begin{aligned} \lambda\frac{dY(\lambda)}{d\lambda} &= \lambda\frac{\partial Y'(\lambda)}{\partial \lambda}|_{\Sigma_\lambda} = \frac{1}{2\beta}Tr(\lambda \widehat{T}_\lambda \widehat{\Lambda}_\lambda) \\ &= \frac{1}{2\beta}Tr(\widehat{T}_\lambda \widehat{\Sigma}_\lambda). \end{aligned} \tag{35}$$

From the equations (20) and (35) we have

$$\lambda\frac{dY(\lambda)}{d\lambda} = \frac{1}{2\beta}Tr(\widehat{T}_\lambda \widehat{\Sigma}_\lambda) = \lambda\frac{dF(\lambda)}{d\lambda}, \tag{36}$$

and we therefore obtain

$$F(\lambda) = Y(\lambda) + F_0, \tag{37}$$

since for $\lambda = 0$ the perturbation is absent $Y(\lambda = 0) = 0$ and $F(\lambda = 0) = F_0$. Now we set $\lambda = 1$ and obtain

$$F = F_0 + Y(1), \tag{38}$$

with the stationarity property

$$\frac{\delta F}{\delta \widehat{\Sigma}} = 0. \tag{39}$$

IV. CONCLUSIONS

We have further developed the diagrammatic theory proposed for strongly correlated systems many years ago to establish the stationarity property of the thermodynamic potential in the superconducting state of the Hubbard model.

First, we have introduced the notion of charge quantum number which gives the possibility to consider the presence of irreducible Green's functions with an arbitrary number of creation or annihilation Fermi- operators in superconducting state.

We have introduced the notion of tunneling Green's function and its mass operator, which turns out to be equal to the correlation function of the fermion system.

We have proven the existence of the Dyson equation for this function and establish the exact relation between the thermodynamic potential and renormalized one-particle propagator. This relation contains an additional integration over the auxiliary constant of interaction λ.

We have constructed a special functional based on the skeleton diagrams for the propagator and for the evolution operator which contain the irreducible Green's functions and full tunneling Green's functions.

We have proven the existence of the stationarity property of this functional and establish its relation with thermodynamic potential.

It is important to emphasize that there is a close similarity between our results obtained for two different models of strongly correlated systems such as Periodic Anderson Model (PAM) and the Hubbard Model (HM). From comparison of the results obtained for the PAM (see paper [17]) and the results of the present paper for the HM the topological coincidence of the diagrams for both models has been revealed.

For example the skeleton diagrams of Fig. 3 of paper [17], obtained for Λ functional of PAM topologically coincide with the skeleton diagrams of our Fig. 2 for the same functional, but of quite a different model. In order to obtain a complete coincidence, it is necessary to replace the full Green's function $G_c(i\omega)$ of conduction electrons of PAM by the renormalized tunneling Green's function $T(i\omega)$ of the HM.

The same similarity exists between other functionals of these models. For example, comparison of the skeleton diagrams of Fig. 10 of paper [17] with the diagrams of Fig. 4 of the present paper reveals the full coincidence upon replacement of the Green's functions G_c by T. This comparison allows us to conclude that from the thermodynamic point of view the Periodic Anderson Model can be reduced to the Hubbard Model if we replace the Green's function of the conduction electrons of PAM subsystem by tunneling Green's function of hopping electrons of HM. This equivalence is irrelevant for the kinetic properties of PAM.

We also note that the skeleton representation of our functional allows to select the local irreducible Green's functions as can be seen from Figs. 2 and 10. These quantities contain only fluctuations in time, unlike the non local ones which include both fluctuations in time and space. The coefficients of local diagrams (see Fig. 10) vary with the order of perturbation theory as $\frac{1}{2^{n-1}n!}$ for $n > 1$.

Only such local diagrams are relevant for DMFT, so that one can attempt to carry out the summation of this class of diagrams.

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Appendix A: Gor'kov-Nambu representation

We consider equation (11) in Fourier representation. By inserting specific values of charge quantum number $\lambda = \pm 1$ we obtain ($k = (\overrightarrow{k}, i\omega_n)$):

$$G^{1,1}_{\sigma\sigma'}(k) = \Lambda^{1,1}_{\sigma\sigma'}(k) + \Lambda^{1,1}_{\sigma\sigma_1}(k)\epsilon_1(\overrightarrow{k})G^{1,1}_{\sigma_1\sigma'}(k) - \Lambda^{1,-1}_{\sigma,-\sigma_1}(k)\epsilon_{-1}(\overrightarrow{k})G^{-1,1}_{-\sigma_1,\sigma'}(k), \tag{A1}$$

$$G^{1,-1}_{\sigma,-\sigma'}(k) = \Lambda^{1,-1}_{\sigma,-\sigma'}(k) + \Lambda^{1,1}_{\sigma\sigma_1}(k)\epsilon_1(\overrightarrow{k})G^{1,-1}_{\sigma_1,-\sigma'}(k) + \Lambda^{1,-1}_{\sigma,-\sigma_1}(k)\epsilon_{-1}(\overrightarrow{k})G^{1,1}_{-\sigma',-\sigma}(-k), \tag{A2}$$

$$G^{-1,1}_{-\sigma,\sigma'}(k) = \Lambda^{-1,1}_{-\sigma,\sigma'}(k) + \Lambda^{-1,1}_{-\sigma,\sigma_1}(k)\epsilon_1(\overrightarrow{k})G^{1,1}_{\sigma_1\sigma'}(k) + \Lambda^{1,1}_{-\sigma_1,-\sigma}(-k)\epsilon_{-1}(\overrightarrow{k})G^{-1,1}_{-\sigma_1,\sigma'}(k), \tag{A3}$$

$$G^{1,1}_{-\sigma',-\sigma}(-k) = \Lambda^{1,1}_{-\sigma',-\sigma}(-k) - \Lambda^{-1,1}_{-\sigma,\sigma_1}(k)\epsilon_1(\overrightarrow{k})G^{1,-1}_{\sigma_1,-\sigma'}(k) + \Lambda^{1,1}_{-\sigma_1,-\sigma}(-k)\epsilon_{-1}(\overrightarrow{k})G^{1,1}_{-\sigma',-\sigma_1}(-k). \tag{A4}$$

Here

$$\epsilon_1(\overrightarrow{k}) = \epsilon(\overrightarrow{k}), \quad \epsilon_{-1}(\overrightarrow{k}) = \epsilon(-\overrightarrow{k}), \quad \epsilon(\overrightarrow{k}) = \frac{1}{N}\sum_{\overrightarrow{x}} t(\overrightarrow{x})e^{i\overrightarrow{k}\overrightarrow{x}}, \quad \sum_{\overrightarrow{k}}\epsilon(\overrightarrow{k}) = 0, \quad G^{-1,-1}_{\sigma\sigma'}(k) = -G^{1,1}_{\sigma'\sigma}(-k). \tag{A5}$$

Assuming that the system is in a paramagnetic state, that superconductivity has a singlet character and using the definitions (8) together with the additional ones:

$$\Lambda^{1,1}_{\sigma\sigma}(k) \;=\; \Lambda_\sigma(k), \Lambda^{1,-1}_{\sigma\overline{\sigma}}(k) = Y_{\sigma\overline{\sigma}}(k),$$

$$\Lambda^{-1,1}_{\overline{\sigma}\sigma}(k) \;=\; \overline{Y}_{\overline{\sigma}\sigma}(k), \tag{A6}$$

we obtain the following results:

$$G_\sigma(k) = \frac{\Lambda_\sigma(k)(1-\epsilon(-\overrightarrow{k})\Lambda_{\overline{\sigma}}(-k)) - \epsilon(-\overrightarrow{k})Y_{\sigma\overline{\sigma}}(k)\overline{Y}_{\overline{\sigma}\sigma}(k)}{d_\sigma(k)}, \quad F_{\sigma\overline{\sigma}}(k) = \frac{Y_{\sigma\overline{\sigma}}(k)}{d_\sigma(k)}, \quad \overline{F}_{\overline{\sigma}\sigma}(k) = \frac{\overline{Y}_{\overline{\sigma}\sigma}(k)}{d_\sigma(k)}, \tag{A7}$$
$$d_\sigma(k) = (1-\epsilon(\overrightarrow{k})\Lambda_\sigma(k))(1-\epsilon(-\overrightarrow{k})\Lambda_{\overline{\sigma}}(-k)) + \epsilon(\overrightarrow{k})\epsilon(-\overrightarrow{k})Y_{\sigma\overline{\sigma}}(k)\overline{Y}_{\overline{\sigma}\sigma}(k),$$

which coincide with those found in the papers[9,10].

In spinor representation the system of equations (A1-A7) has the form

$$\widehat{G} = \widehat{\Lambda} + \widehat{\Lambda}\widehat{\epsilon}\widehat{G}, \tag{A8}$$

were

$$\widehat{G} = \begin{pmatrix} G_\sigma(k) & F_{\sigma\overline{\sigma}}(k) \\ \overline{F}_{\overline{\sigma}\sigma}(k) & -G_{\overline{\sigma}}(-k) \end{pmatrix},$$

$$\widehat{\Lambda} = \begin{pmatrix} \Lambda_\sigma(k) & Y_{\sigma\overline{\sigma}}(k) \\ \overline{Y}_{\overline{\sigma}\sigma}(k) & -\Lambda_{\overline{\sigma}}(-k) \end{pmatrix}, \widehat{\epsilon} = \begin{pmatrix} \epsilon(k) & 0 \\ 0 & -\epsilon(-k) \end{pmatrix} \tag{A9}$$

By using equation (9) we can obtain

$$\begin{aligned} T^{1,1}_\sigma(k) &= \frac{\epsilon(\overrightarrow{k})(1-\epsilon(-\overrightarrow{k})\Lambda_{\overline{\sigma}}(-k))}{d_\sigma(k)}, \\ T^{1,-1}_{\sigma\overline{\sigma}}(k) &= -\epsilon(\overrightarrow{k})\epsilon(-\overrightarrow{k})F_{\sigma\overline{\sigma}}(k), \\ T^{-1,1}_{\overline{\sigma}\sigma}(k) &= -\epsilon(\overrightarrow{k})\epsilon(-\overrightarrow{k})\overline{F}_{\overline{\sigma}\sigma}(k). \end{aligned} \tag{A10}$$